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Conceptual and Computational Analysis of VOC Transport in Ground Water

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ABSTRACT

The aquifers beneath the Lawrence Livermore National Laboratory are contaminated by volatile organic compounds (VOCs) from World War II solvent discharges. These solvent plumes in saturated sediments can be characterized in two regimes: source areas and distal plumes. In distal areas of contaminant plumes, away from the sources, VOCs are essentially limited to coarse-grained zones and are amenable to efficient remediation through existing technology.

Source-area VOC contamination presents a more formidable problem. Here, VOCs are distributed in both fine-grained and coarse-grained zones. Contaminants become essentially trapped in fine-grained zones where there is almost no ground water movement. Their major means of transport out of the fine-grained zones is by the tortuously slow process of molecular diffusion, into the coarse-grained zones where they are advected away. As effective technologies do not exist for the cleanup of deep fine-grained saturated zones, this leakage can continue for centuries, drastically increasing the times and costs of remediation.

Our research focuses on one of the intractable problems in aquifer restoration: managing contaminant transport in and out of fine-grained zones in the source area of a plume. We are adding to our knowledge and ability to remediate these zones through a coupled experimental and computational approach.

We are conducting innovative laboratory column and diffusion experiments investigating the parameters that govern source-area VOC transport: tortuosity (ω), effective diffusion (D^*), and retardation (R_f). Experiments are performed using a low organic carbon, fine grained, well sorted sand and four VOCs commonly found in ground water: tetrachloroethylene, trichloroethylene, carbon tetrachloride, and chloroform. Column experiments revealed that chloroform is not retarded, which led to a potential new method for deriving coefficients describing retardation and tortuosity, using chloroform as a conservative tracer. Also, we discovered that a thin layer of clay on the sand grains greatly effects retardation. To further investigate this important result, all experiments currently use sand with and without this clay layer. Laboratory data is analyzed with parameter estimation software to reduce the uncertainty in values for ω, D^*, and R_f.

Optimal aquifer cleanup requires the ability to simulate VOC transport under various remediation strategies. Our computational approach incorporates laboratory information about ω, D^*, and R_f into state-of-the-art numerical modeling. We use PDEase, advanced adaptive-grid finite element (FEM) software, to solve the transient two-dimensional Advection-Dispersion Equation (ADE) and to evaluate the rate at which VOCs diffuse out of fine-grained zones and into coarse-grained zones during cleanup. Our model represents a two-dimensional vertical cross section of an idealized source area. Where previous research has treated molecular diffusion as insignificant, we see that it plays an important role. Our adaptive-grid model separates hydrodynamic dispersion into its components of molecular diffusion and mechanical dispersion, and more accurately simulates the complexities of source-area VOC transport. PDEase numerical analysis converges to exact solutions and results are consistent with conceptual expectations and field data. We demonstrate in a well-field context that contaminants in fine-grained zones are long-term sources that are difficult to remediate.

Our goal is to continue to improve our understanding of the mechanisms of source-area VOC transport under increasingly realistic geologic and well- field conditions. We hope that the insight and predictive power our project provides will inspire new aquifer remediation technologies. Our refined mathematical tool will be applicable to environmental restoration efforts nationwide.

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